

Isospin coupling in time-dependent-mean-field theories and decay of isovector excitations

C. Simenel^{1,2,3}, Ph. Chomaz², T. Duguet^{3,4}

¹ *DSM/DAPNIA, CEA SACLAY, F-91191 Gif-sur-Yvette, France*

² *GANIL, B.P. 5027, F-14076 CAEN Cedex 5, France*

³ *NSCL, MSU, East Lansing, Michigan 48824, USA and*

⁴ *Physics and Astronomy Department, MSU, East Lansing, Michigan 48824, USA*

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We show that isospin non-diagonal terms should appear in the mean field Hamiltonian when neutron-proton symmetry is broken. They give rise to charge mixing in the single-particle wavefunctions. We study the Time Dependent Hartree-Fock response of a charge-exchange excitation which generates a charge mixing in Ca isotopes. We find an enhancement of the low energy proton emission in neutron-rich isotopes interpreted in terms of a charge oscillation below the barrier.

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Atomic nuclei are a good laboratory to test quantum mechanics of few-body systems. The nucleon-nucleon (NN) interaction can be interpreted in terms of meson exchange and depends on the quantum numbers of the nucleons (spin, isospin, parity...). For instance two protons or two neutrons cannot exchange a single charged pion, unlike a proton-neutron pair. The NN force can be divided into a central, a spin-orbit and a tensor part [1], the latter being mainly mediated by pions. The description of the structure and the dynamic of nuclei through mean-field-like methods [2] makes use of effective interactions such as the Gogny [3] or the Skyrme [4] forces, taking care of both the renormalization of the NN interaction in the medium and of the three-body force. In such models, the residual tensor component is rarely explicitly included but the renormalization of the central and spin-orbit parts by the original tensor, and in particular the saturating effect of the latter, is incorporated on a phenomenological basis through the density dependence and the fitting procedure of the force. This is an important aspect since the tensor force contributes strongly to the binding and spin-orbit splittings of nuclei [5].

However, treated fully or partially, the exchange of charged pions can only be properly accounted for in a mean-field-like theory through the breaking of isospin symmetry of single-particle (s.p.) states. Indeed, including important parts of the residual interaction through breaking of symmetries is a key concept of self-consistent mean-field methods. However, mixing the isospin projection of s.p. states leads to a many-body state with no good charge any more. Such a broken symmetry is to be restored in structure calculations since the nucleus is meant to have isospin projection (i.e. the charge) as a good quantum number. Sugimoto *et al* [6] showed recently that a Hartree-Fock (HF) [7, 8] calculation allowing for the explicit mixing of protons and neutrons (as well as of parity), and followed by the full Variation After Projection technique [9], was indeed a powerful tool to include correlations associated with the explicit treatment of the tensor force. Such involved calculations can only be applied to very light nuclei however. Also, the

complete Hartree-Fock-Bogoliubov (HFB) formalism including charge mixing in both the particle-hole (p-h) and the particle-particle (p-p) channels was derived recently by Perlińska *et al* [10] within the Density Functional Theory framework. In this context, both the neutron-proton pairing and the correlations associated with the tensor force in the p-h channel could be studied. However, no calculation has been performed so far.

Symmetry breaking can also affect reaction mechanisms. When correctly introduced and restored in the initial state, it may account for the propagation of ground-state correlations. Moreover, reactions may induce an explicit symmetry breaking. For instance, the wave function of one of the collision partners in a Charge-Exchange (CE) reaction becomes a superposition of isobaric nuclei. While the wave function describing both collision partners has to conserve charge exactly, both nuclei are entangled after the collision, i.e. the wave function obtained by projection on one of the two separated products have not a good isospin before any detection takes place. Each component of the isospin T_3 affects the evolution of the others through the non linearities of the mean field.

Mean-field methods should be generalized to take into account such dynamical symmetry breaking induced by the reaction. The aim of the present letter is to include, for the first time, isospin-symmetry breaking in Time-Dependent Hartree-Fock (TDHF) calculations [11] within the Skyrme energy functional framework. As a first application, the effect of correlations associated with s.p. isospin mixing on the nucleon emission following a CE excitation are studied.

In mean-field methods, allowing for s.p. isospin mixing translates into the appearance of non-diagonal terms in the HF Hamiltonian in isospin space. We derive such terms starting from an effective Skyrme interaction [2]:

$$\begin{aligned}
\hat{v} = & t_0(1+x_0\hat{P}_\sigma)\hat{\delta} + \frac{t_1}{2}(1+x_1\hat{P}_\sigma)\left(\hat{\delta}\hat{\mathbf{k}}^2 + \hat{\mathbf{k}}'^2\hat{\delta}\right) \\
& + t_2(1+x_2\hat{P}_\sigma)\hat{\mathbf{k}}'\cdot\hat{\delta}\hat{\mathbf{k}} + \frac{t_3}{6}(1+x_3\hat{P}_\sigma)\rho^\beta(\hat{\mathbf{R}}_{12})\hat{\delta} \\
& + iV_{so}(\hat{\sigma}_1 + \hat{\sigma}_2)\cdot\hat{\mathbf{k}}'\times\hat{\delta}\hat{\mathbf{k}}, \quad (1)
\end{aligned}$$

where $\hat{\delta} = \delta(\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2)$, $\hat{\mathbf{R}}_{12} = (\hat{\mathbf{r}}_1 + \hat{\mathbf{r}}_2)/2$, $\hat{\mathbf{k}} = \frac{\hat{\nabla}_1 - \hat{\nabla}_2}{2i}$ acts on the right, while its Hermitian conjugated $\hat{\mathbf{k}}'$ acts on the left and $\hat{P}_\sigma = \frac{1}{2}(1 + \hat{\sigma}_1\hat{\sigma}_2)$ is the spin exchange operator. In Eq. (1) $\rho(\hat{\mathbf{r}})$ is the total local density defined from the one-body density matrix $\langle \mathbf{r}sq|\hat{\rho}|\mathbf{r}'s'q' \rangle = \sum_h \varphi_h^*(\mathbf{r}'s'q')\varphi_h(\mathbf{r}sq)$, where $\varphi_h(\mathbf{r}sq) = \langle \mathbf{r}sq|h \rangle$ denotes the component with a spin s and isospin q of the occupied s.p. wave-function h . It is convenient to decompose $\hat{\rho}$ into its spin-isospin components acting only in coordinate space:

$$\hat{\rho}_{\alpha\mu} = \sum_{ss'qq'} \langle sq|\hat{\rho}|s'q' \rangle \langle s|\hat{\sigma}_\alpha|s' \rangle \langle q|\hat{\tau}_\mu|q' \rangle, \quad (2)$$

where the α index relates to the spin degree of freedom and μ to the isospin one (γ or η are kept for the 3D-space). Whenever α (μ) is 0, only the scalar (isoscalar) part of the density is considered, i.e. $\hat{\sigma}_\alpha$ ($\hat{\tau}_\mu$) is replaced by the identity, $\hat{\sigma}_0 = 1_s$ ($\hat{\tau}_0 = 1_q$). In Eq. (2), densities with $\mu = 1, 2$ are non-diagonal in isospin and will then describe the charge mixing. The HF ground-state energy associated with the Skyrme force defined in Eq. (1) can be written as an integral of a local energy density $\mathcal{H}(\mathbf{r})$ which is a functional of the spin-isospin local densities $\rho_{\alpha\mu}(\mathbf{r}) = \langle \mathbf{r}|\hat{\rho}_{\alpha\mu}|\mathbf{r} \rangle$, kinetic densities $T_{\alpha\mu}(\mathbf{r}) = \left[\sum_\gamma \nabla_\gamma \nabla'_\gamma \langle \mathbf{r}|\hat{\rho}_{\alpha\mu}|\mathbf{r}' \rangle \right]_{\mathbf{r}=\mathbf{r}'}$ and current densities $J_{\gamma\alpha\mu}(\mathbf{r}) = \frac{1}{2i} [(\nabla_\gamma - \nabla'_\gamma) \langle \mathbf{r}|\hat{\rho}_{\alpha\mu}|\mathbf{r}' \rangle]_{\mathbf{r}=\mathbf{r}'}$. In order to shorten the equations, the \mathbf{r} dependence is not written explicitly in the following. The contributions to \mathcal{H} associated with t_0 , t_1 , t_2 and t_3 terms in Eq. (1) have similar structures:

$$\mathcal{H}_k = C_k \sum_{\alpha,\mu=0}^3 d_k^{\alpha\mu} \mathcal{F}_k^{\alpha\mu},$$

with $d_2^{00} = 5+4x_2$, $d_2^{\alpha 0}|_{\alpha \neq 0} = d_2^{0\mu}|_{\mu \neq 0} = 2x_2+1$, $d_2^{\alpha\mu}|_{\alpha\mu \neq 0} = 1$ and, for $k \in \{0, 1, 3\}$, $d_k^{00} = 3$, $d_k^{\alpha 0}|_{\alpha \neq 0} = 2x_k-1$, $d_k^{0\mu}|_{\mu \neq 0} = -2x_k-1$ and $d_k^{\alpha\mu}|_{\alpha\mu \neq 0} = -1$. The functions $C_k(\mathbf{r})$ are defined by $C_0 = \frac{t_0}{8}$, $C_1 = \frac{-t_1}{64}$, $C_2 = \frac{t_2}{64}$, $C_3 = \frac{t_3}{48}\rho_{00}^\beta$ and the functionals \mathcal{F} by $\mathcal{F}_0^{\alpha\mu} = \mathcal{F}_3^{\alpha\mu} = \rho_{\alpha\mu}^2$,

$$\mathcal{F}_1^{\alpha\mu} = 3\rho_{\alpha\mu}\Delta\rho_{\alpha\mu} - 4\rho_{\alpha\mu}T_{\alpha\mu} + 4J_{\gamma\alpha\mu}^2,$$

and $\mathcal{F}_2^{\alpha\mu} = 4\rho_{\alpha\mu}\Delta\rho_{\alpha\mu} - \mathcal{F}_1^{\alpha\mu}$. The spin-orbit term is:

$$\mathcal{H}_{so}[\hat{\rho}] = \frac{-V_{so}}{4} \sum_{\mu=0}^3 d_{so}^\mu \mathcal{F}_{so}^\mu, \quad (3)$$

with $d_{so}^\mu = 1 + 2\delta_{\mu 0}$ and

$$\mathcal{F}_{so}^\mu = \sum_{\gamma\eta\alpha=1}^3 \varepsilon_{\gamma\eta\alpha} (J_{\gamma 0\mu} \nabla_\eta \rho_{\alpha\mu} + J_{\gamma\alpha\mu} \nabla_\eta \rho_{0\mu}),$$

where $\varepsilon_{\gamma\eta\alpha}$ is the antisymmetric tensor.

The HF Hamiltonian is obtained through the functional derivative $\hat{h}[\hat{\rho}] = \partial E[\hat{\rho}]/\partial \hat{\rho}^T$. One expresses the variation of the energy through the variation of the various local densities defined above. One can show in the same way as in Ref. [12] that their contributions to the HF Hamiltonian are $\delta\rho_{\alpha\mu} \rightarrow \hat{\sigma}_\alpha \hat{\tau}_\mu$, $f\delta T_{\alpha\mu} \rightarrow -\hat{\sigma}_\alpha \hat{\tau}_\mu \sum_\gamma \hat{\nabla}_\gamma f \hat{\nabla}_\gamma$ and $f\delta J_{\gamma\alpha\mu} \rightarrow \frac{1}{2i} \hat{\sigma}_\alpha \hat{\tau}_\mu (\hat{\nabla}_\gamma f + f \hat{\nabla}_\gamma)$ where the $\hat{\nabla}$ operators act on each term sitting on their right, including the wave functions. Finally the HF Hamiltonian reads as:

$$\begin{aligned}
\hat{h} = & -\frac{\hbar^2}{2m} \hat{\Delta} + \frac{\beta}{\rho} \mathcal{H}_3 + 2 \sum_{k,\alpha,\mu=0}^3 C_k d_k^{\alpha\mu} \hat{\sigma}_\alpha \hat{\tau}_\mu \hat{G}_k^{\alpha\mu} \\
& - \frac{V_{so}}{4} \sum_{\alpha=1,\mu=0}^3 d_{so}^\mu \hat{\tau}_\mu (\hat{G}_{so}^{\alpha\mu} + \hat{\sigma}_\alpha \hat{G}_{so}^{0\mu}), \quad (4)
\end{aligned}$$

with the operators \hat{G} given by $\hat{G}_0^{\alpha\mu} = \hat{G}_3^{\alpha\mu} = \rho_{\alpha\mu}$, $\hat{G}_2^{\alpha\mu} = 4\Delta\rho_{\alpha\mu} - \hat{G}_1^{\alpha\mu}$ and

$$\begin{aligned}
\hat{G}_1^{\alpha\mu} = & 3\Delta\rho_{\alpha\mu} - 2T_{\alpha\mu} \\
& + \sum_\gamma 2\hat{\nabla}_\gamma \rho_{\alpha\mu} \hat{\nabla}_\gamma - 2i(\hat{\nabla}_\gamma J_{\gamma\alpha\mu} + J_{\gamma\alpha\mu} \hat{\nabla}_\gamma) \\
\hat{G}_{so}^{\alpha\mu} = & \sum_{\gamma\eta} \varepsilon_{\gamma\eta\alpha} \left(\frac{1}{2i} (\hat{\nabla}_\gamma \partial_\eta \rho_{\alpha\mu} + \partial_\eta \rho_{\alpha\mu} \hat{\nabla}_\gamma) - \partial_\eta J_{\gamma\alpha\mu} \right),
\end{aligned}$$

where the derivative ∂_γ and Δ acts only on the function next to them. Everything derived above is valid both for HF and TDHF calculations which corresponds to $[\hat{h}[\hat{\rho}(t)], \hat{\rho}(t)] = i\hbar \partial_t \hat{\rho}(t)$ [12].

The breaking of the isospin symmetry leads to a non diagonal \hat{h} in isospin space because of the $\hat{\tau}_{1,2}$ operators in Eq.(4). Through the dynamics, such a non-diagonal Hamiltonian will lead to an isospin oscillation analogous to the Larmor precession of spins in an unaligned magnetic field or to particle oscillation in a non diagonal mass operator. In order to quantitatively illustrate the phenomenon of isospin mixing in the case of a CE excitation, let us use a simplified version of the complete Skyrme force introduced in Eq. (1):

$$\hat{v} = (f[\rho_{00}] + f_\sigma[\rho_{00}]\hat{P}_\sigma) \hat{\delta}, \quad (5)$$

with $f[\rho_{00}] = t_0 + \frac{t_3}{6}\rho_{00}^\beta$ and $f_\sigma[\rho_{00}] = t_0 x_0 + \frac{t_3}{6} x_3 \rho_{00}^\beta$. The parameters $t_0 = -1803.38 \text{ MeV.fm}^3$ and $t_3 =$

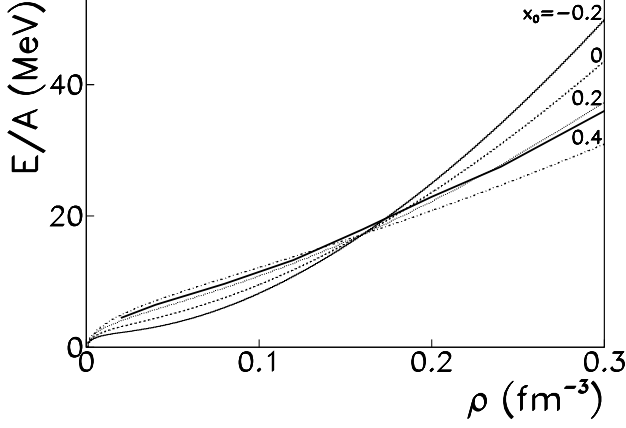


FIG. 1: EoS of pure neutron matter. Variational calculation with Eq. (5) with different values of x_0 .

12912.80 MeV.fm $^{3(1+\beta)}$ have been adjusted to reproduce the empirical saturation point of infinite symmetric matter whereas $\beta = 1/3$ was chosen to have a reasonable compressibility $K_\infty = 236.2$ MeV. As momentum-dependent and spin-orbit terms are dropped, the nucleon effective mass m^* is equal to the bare one and the scalar time odd current density is not generated by the force, while spin-orbit splittings and some magic numbers are not reproduced in finite nuclei. Asking for a value of the symmetry energy $a_s = 32.5$ MeV at saturation density $\rho_{sat} = 0.16$ fm $^{-3}$ gives the relation $x_3 = 1.544 x_0 + 0.161$. Different values of x_0 were tried in order to match the Equation of State (EoS) of infinite neutron matter predicted by Akmal *et al.* through variational chain summation methods [13] (thick-solid line on Fig. 1). The value of $x_0 = 0.2$ for which the EoS of neutron matter obtained from microscopic calculations is well reproduced was finally used (see Fig. 1). In view of the commonly accepted value chosen the symmetry energy and the fair reproduction of the EoS of neutron matter, one can expect the isovector properties of the simplified Skyrme force and the isospin mixing arising from it to be reasonable. In addition, the proton and neutron separation energies are close to the experimental values for the ^{40}Ca : $S_p = 8.25$ MeV and $S_n = 16.56$ MeV. However, going far from stability the separation energies are not as good. For ^{60}Ca , a HFB-Lipkin-Nogami calculation gives $S_p = 24.33$ MeV and $S_n = 3.57$ MeV [14] whereas we get $S_p = 19.35$ MeV and $S_n = 8.38$ MeV. The full Skyrme force of Eq. 1 is needed to correct for this discrepancy.

We now write the TDHF potential associated with the force in Eq. (5), focusing on even-even nuclei. In their ground state, only time-reversal invariant local densities are non-zero. Thus, s.p. states with a good spin can be used. This remains true during the dynamical evolution as long as we do not break explicitly the spin symmetry in the wave function. With this hypothesis, all terms with a α index vanish in Eq. (4). Finally, we are left

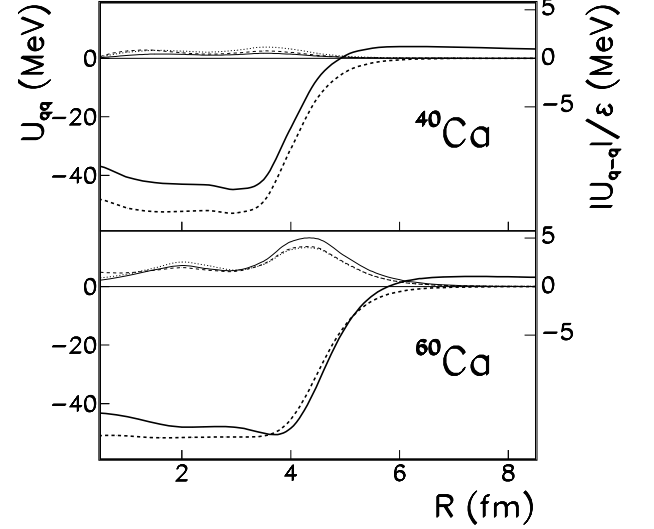


FIG. 2: Proton (thick solidline) and neutron (thick dashed line) diagonal potentials U_{qq} and isospin coupling modulus $|U_{q-q}|$ divided by the boost strength ε at 30, 360 and 690 fm/c (thin solid, dashed and dotted lines respectively) for non spin-flip CE excitations in ^{40}Ca (up) and ^{60}Ca (down).

with the potential matrix elements:

$$\begin{aligned}
 U_{qq} &= \frac{3}{8} \frac{\partial}{\partial \rho_{00}} (f \rho_{00}^2) - \frac{1}{8} \left(4q \rho_{03} + \sum_{\mu=1}^3 \rho_{0\mu}^2 \frac{\partial}{\partial \rho_{00}} \right) \\
 &\quad (f + 2f_\sigma) + \delta_{q, \frac{1}{2}} U_c \\
 U_{q-q} &= -\frac{1}{4} (f + 2f_\sigma) \eta_q,
 \end{aligned} \tag{6}$$

where U_c is the Coulomb potential. The non-diagonal part U_{q-q} , or “isospin coupling” is proportional to the isospin mixing density, $\eta_q = \frac{1}{2} \rho_{01} + i q \rho_{02} = \sum_s \langle \mathbf{r} s q | \hat{\rho} | \mathbf{r} s - q \rangle$. We can now study a non spin-flip CE excitation generated by a collective isovector boost applied at $t = 0$ to an isospin-diagonal HF ground state $|\phi_0\rangle$: $|\phi(0)\rangle = e^{-i\varepsilon \hat{\tau}_u} |\phi_0\rangle$ where ε and \mathbf{u} denote the boost strength and direction in isospin space, respectively. When \mathbf{u} is not aligned with the $\hat{\tau}_3$ axis, a CE takes place and $|\phi(0)\rangle$ is then an antisymmetrized product of s.p. wave-functions which mixed protons and neutrons. For $N = Z$ nuclei the CE produced is quenched by the Pauli principle (and vanishes if Coulomb is neglected). As explained earlier, the wave function after the CE excitation is a linear combination of isobaric analog nuclei. The influence on the dynamics of such a quantum entanglement in isospin space is incorporated in the TDHF method developed in the present letter.

We have computed numerically the TDHF evolution after a boost an isovector applied on the ground state of ^{40}Ca and ^{60}Ca . The simplified Skyrme mean field Eq. (6) is considered. If $\varepsilon \ll 1$, the diagonal potentials (U_{qq}) are almost constant in time while the isospin coupling is

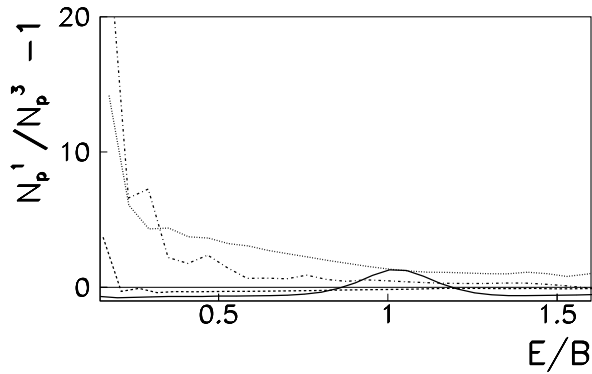


FIG. 3: Ratio of the numbers of emitted proton following an isovector excitation by the τ_1 and τ_3 operators as function of the proton energy E divided by the barrier B for the $^{40-48-54-60}\text{Ca}$ (solid, dashed, dotted, dotted-dashed lines respectively).

linear in ε . The resulting potentials at different times are plotted in Fig. 2. The small variation in time of $|U_{q-q}|$ comes from the difference in energy of the excited modes. $|U_{q-q}|$ is more intense in ^{60}Ca than in ^{40}Ca as expected from the quenching of CE processes in the $N=Z$ nuclei. The isospin coupling is also more peaked at the surface in ^{60}Ca because of the isospin mixing in the $2p-1f$ shells and decreases exponentially at the barrier.

Let us now present a possible effect of the isospin coupling on the low energy proton emission. The particle emission looked at in the present case originates from the entangled state prior to any detection of the reaction partner (\Leftrightarrow projection on good isospin). An emitted proton (neutron) can come from an incident proton (neutron) or an incident neutron (proton) which has exchanged its isospin via the isospin coupling. At low energy, where the proton emission is hindered by the Coulomb barrier, one can expect an enhancement of the proton emission from neutron which exchange their isospin at the surface. This is possible because the isospin coupling does not fully vanish at the surface (see Fig. 2). The excitation studied above does not usually populate states above the nucleon threshold. To reach such high excitation energy we applied on the HF ground state an isovector-monopole boost $e^{-i\varepsilon\hat{r}^2\hat{\tau}_u}$. Due to the \hat{r}^2 oper-

ator, an important part of the strength goes to the $2\hbar\omega$ non spin-flip Isovector Giant Monopole Resonance. Let us compare the numbers of protons emitted at an energy E after a boost generated by τ_3 (noted N_p^3) and by τ_1 (N_p^1). Fig. 3 shows the evolution of $N_p^1/N_p^3 - 1$ obtained for $^{40-48-54-60}\text{Ca}$. We choose $\varepsilon = 0.01 \text{ fm}^{-2}$ which is small enough to be in the linear regime.

For a τ_3 -boost, there is no isospin coupling whereas a τ_1 excitation produces an isospin coupling slightly more peaked at the surface than in Fig. 2 due to the r^2 term in the boost. In this case the expectation value of the charge is changed by $\Delta\langle Z \rangle = -0.0044$ in ^{40}Ca and 0.064 in ^{60}Ca . Fig. 3 shows a strong enhancement of the proton emission at energies well below the barrier except for the ^{40}Ca for which the isospin coupling remains small. Around the barrier this effect is hindered by the difference in the excitation energy spectra associated with the inelastic and the charge exchange excitations. This enhancement of the low energy proton is expected to be a general consequence of isospin coupling. In fact we expect this effect to be strong in all nuclei with large proton/neutron asymmetry.

To conclude, we have shown that isospin coupling appears in the HF mean field when proton-neutron symmetry is broken. Its expression was derived for a full Skyrme-like force. We used a simplified Skyrme force adjusted on the isospin properties of nuclear matter to get an approximation of the isospin mixing. As a first application we performed TDHF calculations using this force to study the effect of charge-exchange excitations on nucleon emission. We found an enhancement of the proton emission below the barrier for the neutron rich Ca interpreted in terms of nucleon charge oscillation. More quantitative predictions are needed with a 3D-TDHF code with a full Skyrme force to study complete reactions, i.e. not only the evolution of one nucleus wave function. The inclusion of the spin degree of freedom would also allow studies of Gamow-Teller transitions and isospin and spin-flip giant resonances. For the latter case however and for any nuclear structure study in general, it is necessary to keep the good value of the charge in average during the time evolution and to project on it after.

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